Co-Optimization of Fuels & Engines

Opportunities for High-Value Bioblendstocks to Enable Advanced Light- and Heavy-Duty Engines: Insights from the Co-Optima Project

TRB 2018 Annual Meeting

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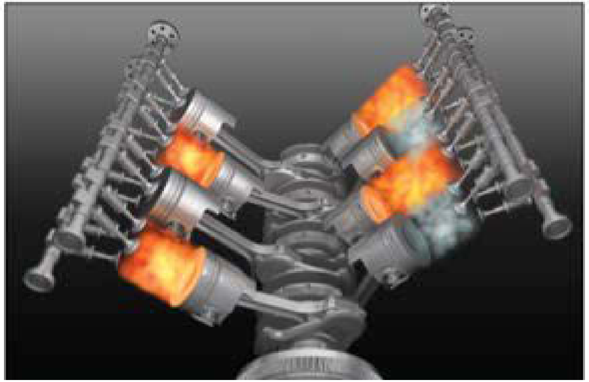
Co-Optima Leadership Team:

John Farrell (NREL), John Holladay (PNNL),
Robert Wagner (ORNL), Chris Moen (SNL)

Overview of Today's Presentations

What fuels do engines *really* want?	What fuels *should* we make?	What will work in the real world?
		

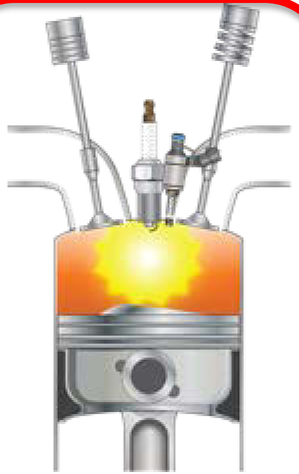
Goal: better fuels and better vehicles sooner

Fuel and Engine Co-Optimization

- What fuel properties maximize engine performance?
- How do engine parameters affect efficiency?
- What fuel and engine combinations are sustainable, affordable, and scalable?

Two Parallel R&D Projects

Light-Duty



Boosted SI

Higher efficiency via downsizing

Near-term

Multi-mode SI/ACI

Even higher efficiency over drive cycle

Mid-term

Medium/Heavy-Duty

Mixing Controlled

Improved engine emissions

Near-term

Kinetically Controlled

Highest efficiency and emissions performance

Longer-term

High-level goals and outcomes

Light-duty

10% fuel economy (FE) improvement* from boosted SI and multi-mode SI/ACI

Heavy-duty

Up to 4% FE improvement (worth $5B/year)*

Potential lower cost path to meeting next tier of criteria emissions regulations

Fuels

Diversifying resource base

Providing economic options to fuel providers to accommodate changing global fuel demands

Increasing supply of domestically sourced fuel by up to 25 billion gallons/year

Cross-cutting goals

Stimulate domestic economy

Adding up to 500,000 new jobs

Providing clean-energy options

* Beyond projected results of current R&D efforts; 2030 target. The team is actively engaging with OEMs, fuel providers, and other key stakeholders to refine goals and approaches to measuring fuel economy improvements

Co-Optima Team

Nine national labs,
13 universities

> 100 researchers,
> 75 projects

External Advisory Board

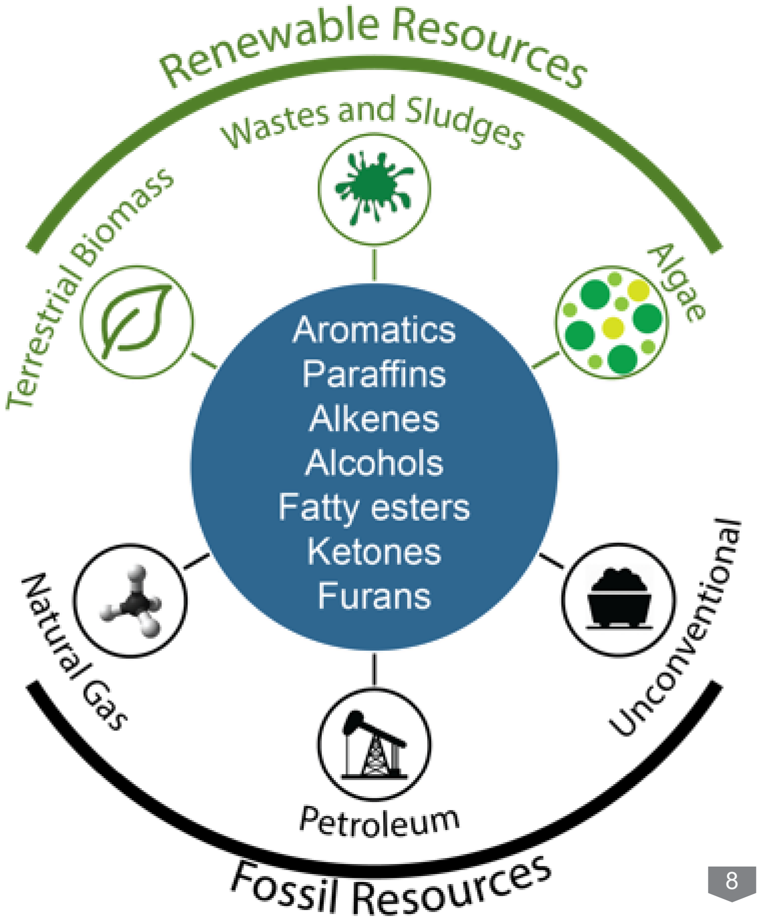
77 stakeholder organizations

Budget: FY16: $26M
FY17: $24.5
Universities: $7M/3 years

Approach

Objective: identify fuel properties that optimize engine performance, independent of composition,* allowing the market to define the best means to blend and provide these fuels

* We are not going to recommend that any specific blendstocks be included in future fuels

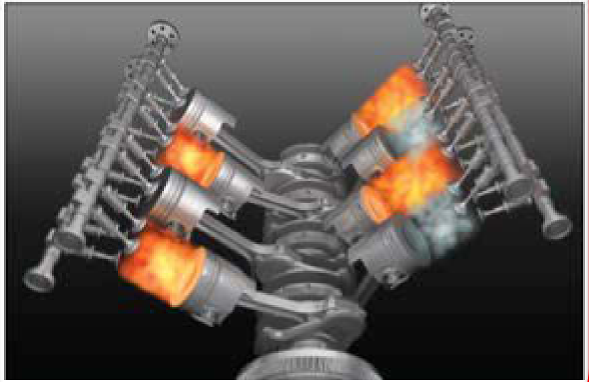


Research Approach to Maximizing Bioblendstock Value

- Determine fuel properties most effective at improving the efficiency of advanced LD and HD engines
- Establish fundamental understanding of how properties are governed by molecular structure
- Outline pathways for producing these blendstocks from domestic cellulosic biomass and similar renewable, non-food, and surplus waste resources
- Identify key research challenges that must be overcome to address economic, environmental, technology, and market barriers

Foundational Technical Questions

What fuels do engines *really* want?



What fuels *should* we make?

What will work in the real world?

Question 1: What fuels do engines really want?

Approach:

Conduct engine experiments and simulations that delineate fuel property impacts on engine performance

Focus: boosted SI engines

Fuel Properties Impacting Boosted SI Efficiency

Octane Index (Knock) — RON, Octane Sensitivity

Charge Cooling — Heat of Vaporization

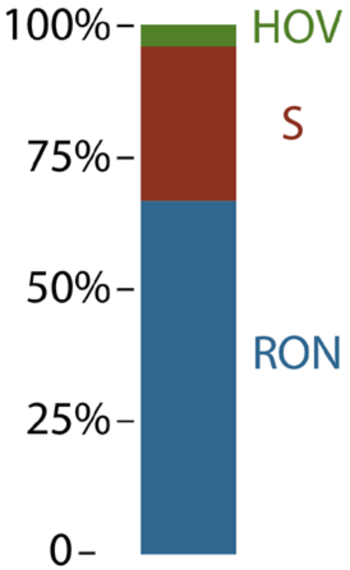
$$\text{Merit (efficiency)} = \alpha \bullet f(\text{RON}) + \beta \bullet f(K, S) + \gamma \bullet f(\text{HOV}) + \varepsilon \bullet f(\text{LFS}) + \zeta \bullet f(\text{PMI}) + \eta \bullet f(T_{c,90,conv})$$

Flame Speed — PM Emissions — Catalyst Light-off Temp (cold start)

Burn Rate/ Dilution Tolerance

Emissions Penalties

Average contribution to merit function for highest scoring blendstocks



Foundational Technical Questions

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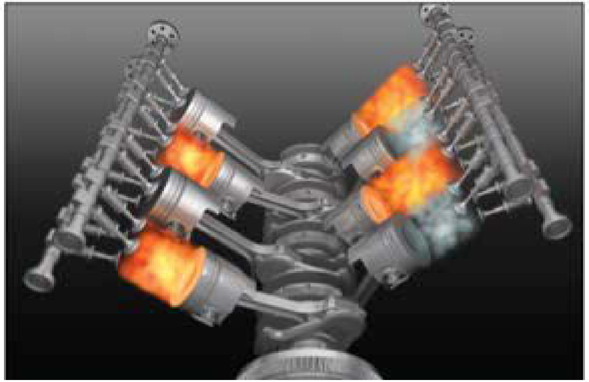


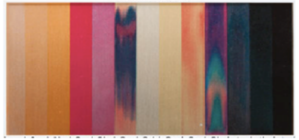
What fuels *should* we make?

What will work in the real world?

Fuel-Property Based Approach

Rigorous Screening

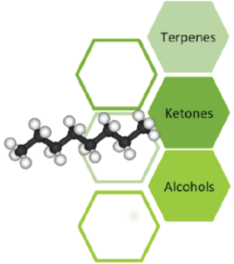
Rapidly identify viable candidates



Blendstock Evaluation

Measure properties

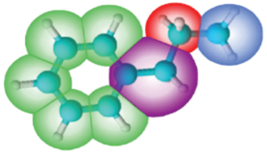
Populate database

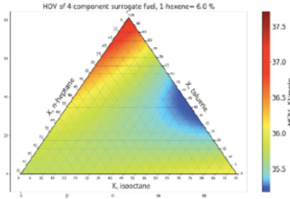


Generate Insight

Develop blending models

Correlate properties to molecular structure

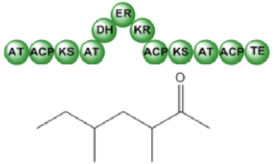


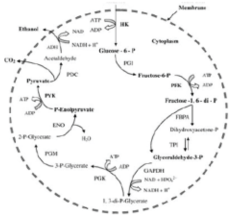


Establish Bio Pathways

Target properties to generate key data

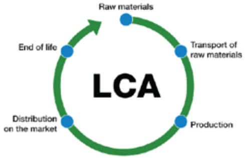
Conduct retrosynthetic analyses

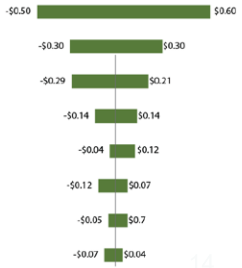




Inform Analyses

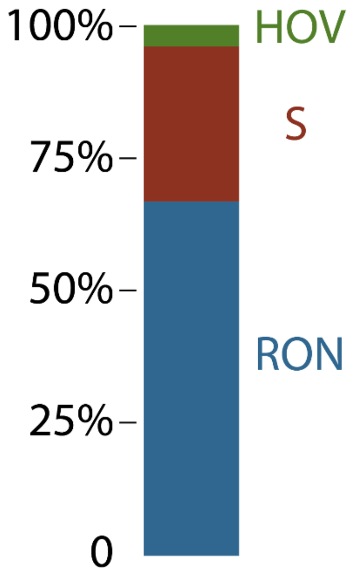
Provide improved data for LCA, TEA analyses





Current Boosted SI Blendstock Evaluation

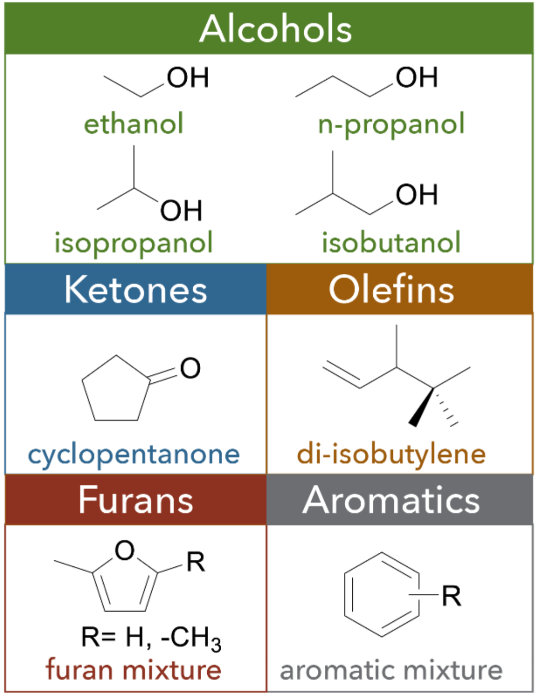
Average contribution to merit function for highest scoring blendstocks



Properties provided by chemical families:

	RON	S	HOV
Alcohols	✔	✔	✓
Furans	✔	✔	
Alkenes	✔	✔	
Aromatics	✔	✔	
Ketones	✔	✔	
Cycloalkanes	✔	✓	
Esters	✔	✓	
Alkanes	✔		
Ethers	✔		

Blendstocks from 5 chemical families selected for more detailed evaluation



RON = Research octane number ; S = Sensitivity (S = RON – MON) ; HOV = heat of vaporization

Tool Highlight: Feature Creature

Question: How do you make a given blendstock from biomass?

Approach:

- Retrosynthetic analysis: reverse engineering process to synthesize a desired product
  - 1^{st} systematic fuel property-based approach
- Identified one or more biochemical and thermochemical pathways for more than 40 high-potential blendstocks
- Provides basis to evaluate conversion pathways, identify gaps, and inform analysis efforts
- Provides pathways for evaluation, and basis for determining whether additional pathway development is necessary

Tool Highlight: Retrosynth

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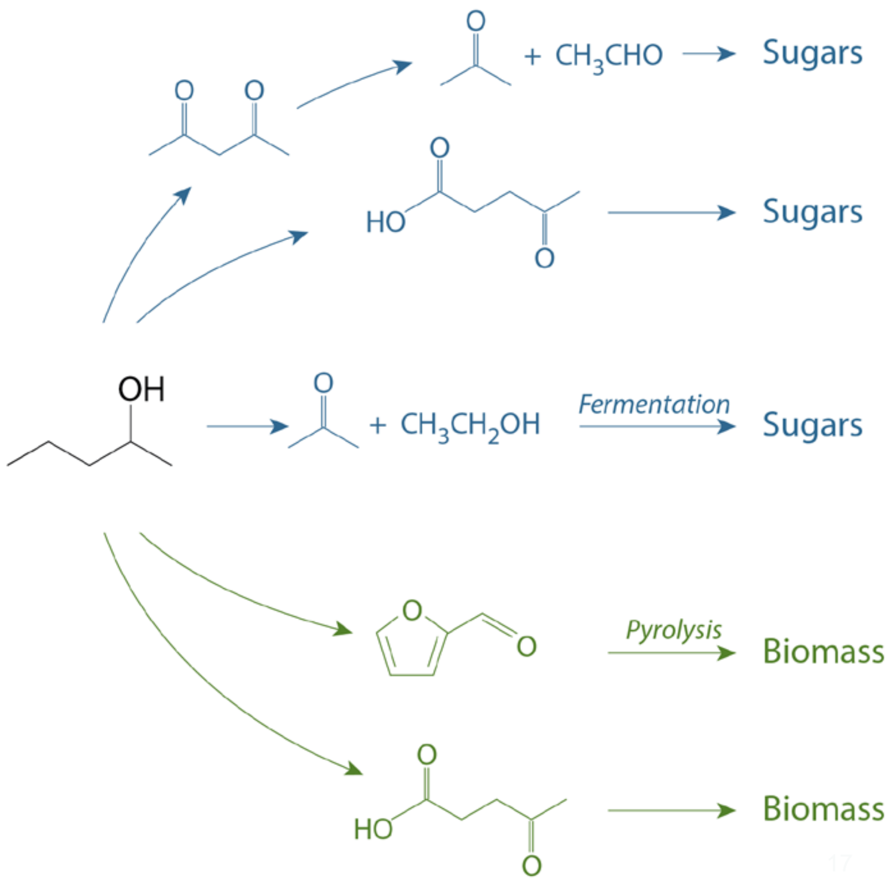
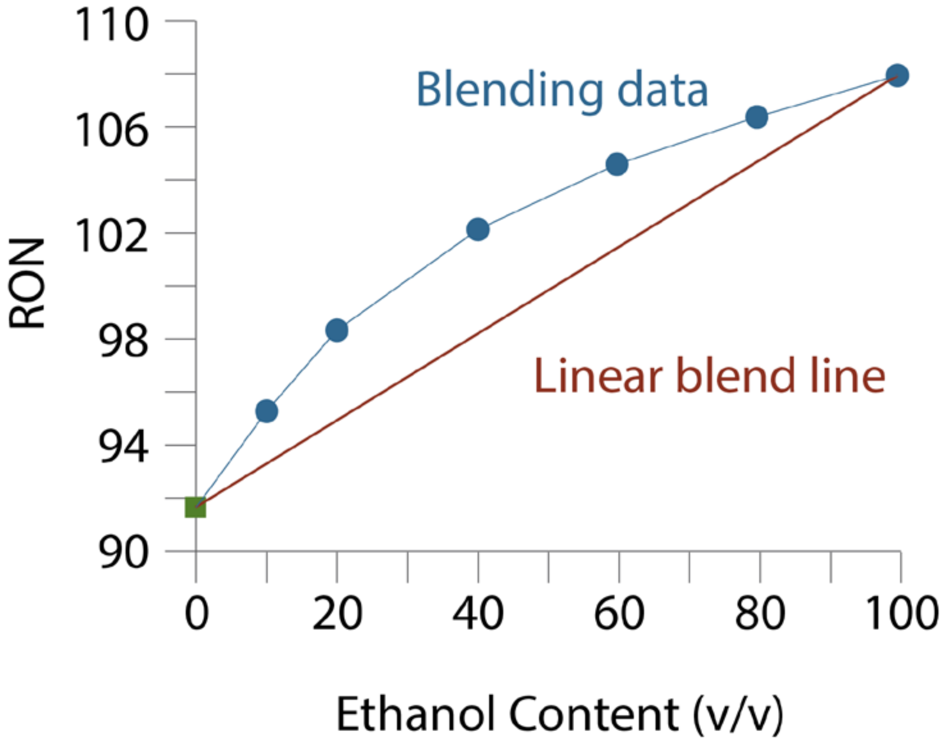
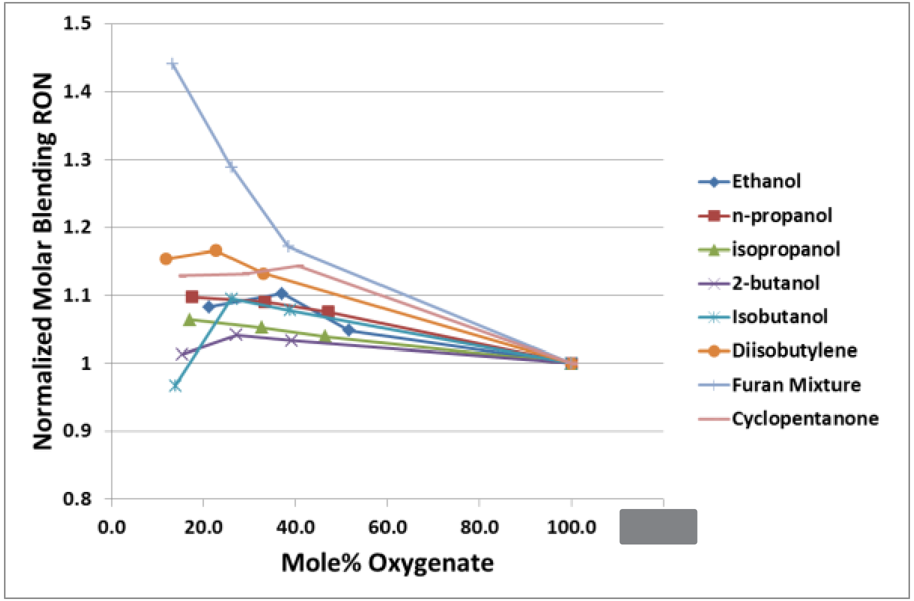


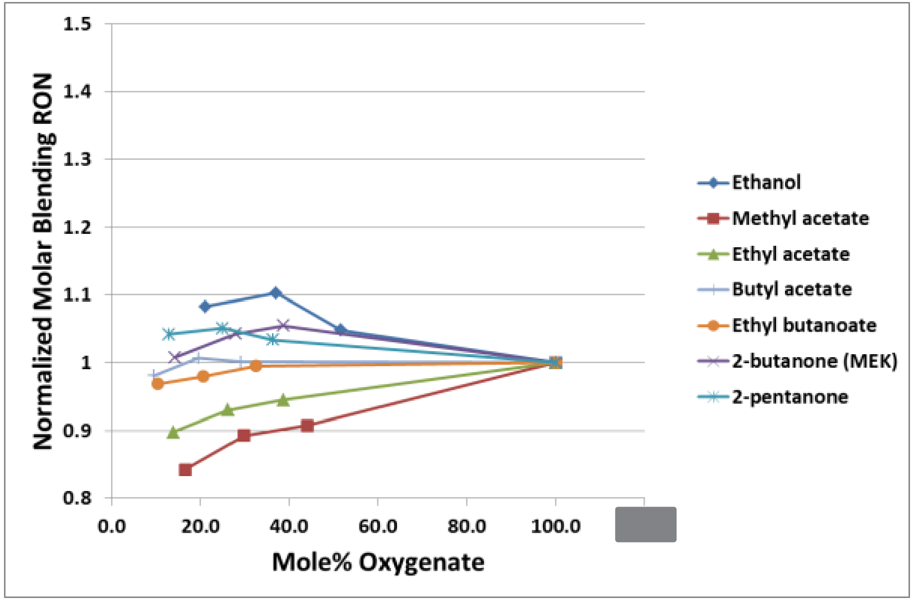
Understanding Blending Effects

- Many blendstocks exhibit beneficial non-linear blending behavior
  - "Effective" blending number is higher than pure component's
- Value proposition:
  - Determine molecular basis for non-linear RON and S blending
  - Identify bioblendstocks with greatest potential to impart advantageous properties



Bioblendstocks – RON Blending Behavior

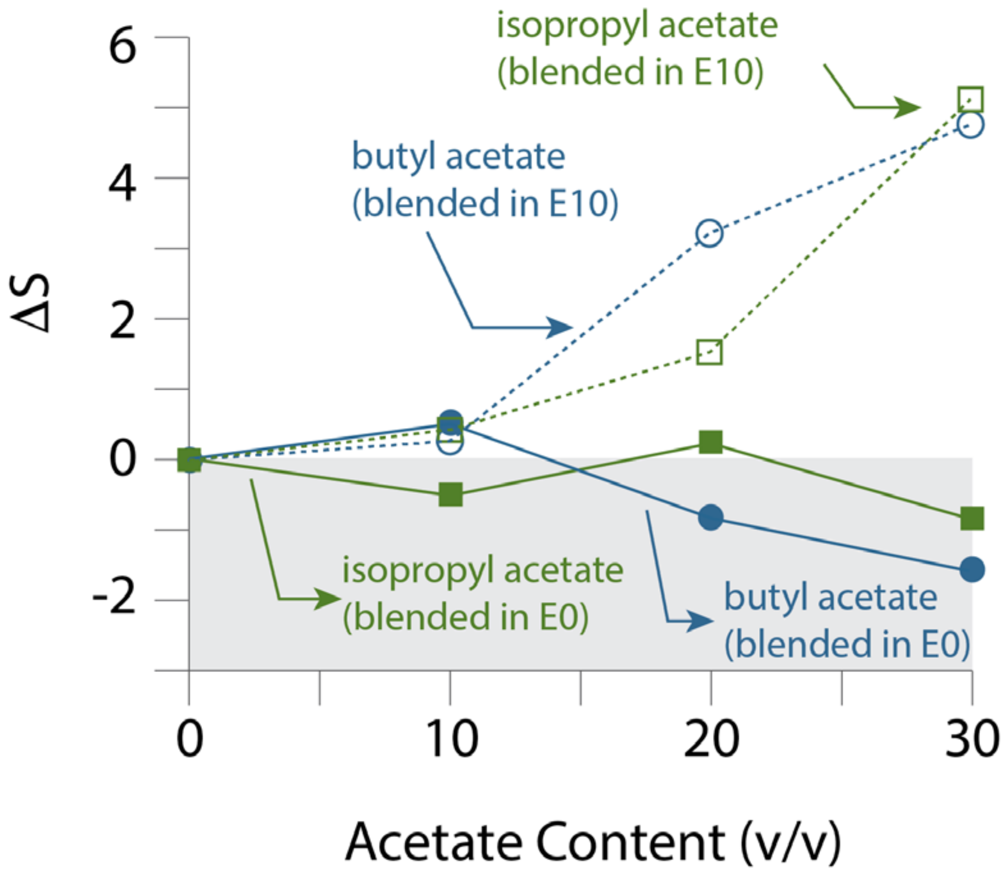




- Comprehensive blending studies in gasoline surrogate w/ and w/o ethanol
- Non-linear blending is norm
  - May be either synergistic (furans) or antagonistic (esters)

Ester Sensitivity Enhanced with Ethanol

- Esters are high-RON, low S blendstocks
- Esters blended into E0 impart no octane sensitivity
- Blending into E10 “turns on” S
- Value proposition:
  - Identify mechanism behind ethanol enhancement
  - Identify bioblendstocks that synergistically blend with ethanol to yield high S

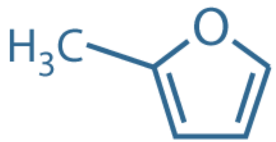


Furans as Gasoline Blending Components

Beneficial Properties

Beneficial Properties	Furans*	Ethanol	Higher Alcohols**
Readily produced from biomass	✔	✔	✔
High blending RON	✔ (145)	✔ (144)	✔ (117-129)
High octane sensitivity	✔ (15)	✔ (12)	✔ (12-15)
High lower heating value (MJ/liter)	✔ (32.2)	(20.2)	✓ (24-27)
Low water solubility (g/liter)	✔ (2.2)	(∞)	✓ (0.9 - ∞)
Minimal impact on fuel volatility	✔		✓

* 40:60 blend of MF:DMF (by weight) ** iso-propanol, n-propanol, iso-butanol



2-methylfuran (MF)

2,5-dimethylfuran (DMF)

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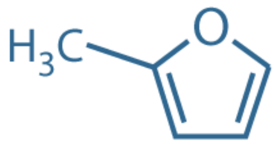


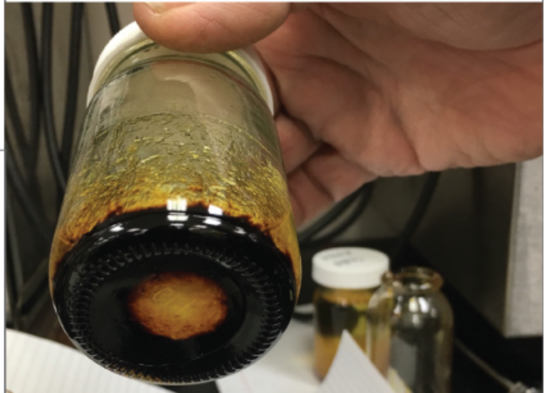
2-methylfuran (MF)

2,5-dimethylfuran (DMF)

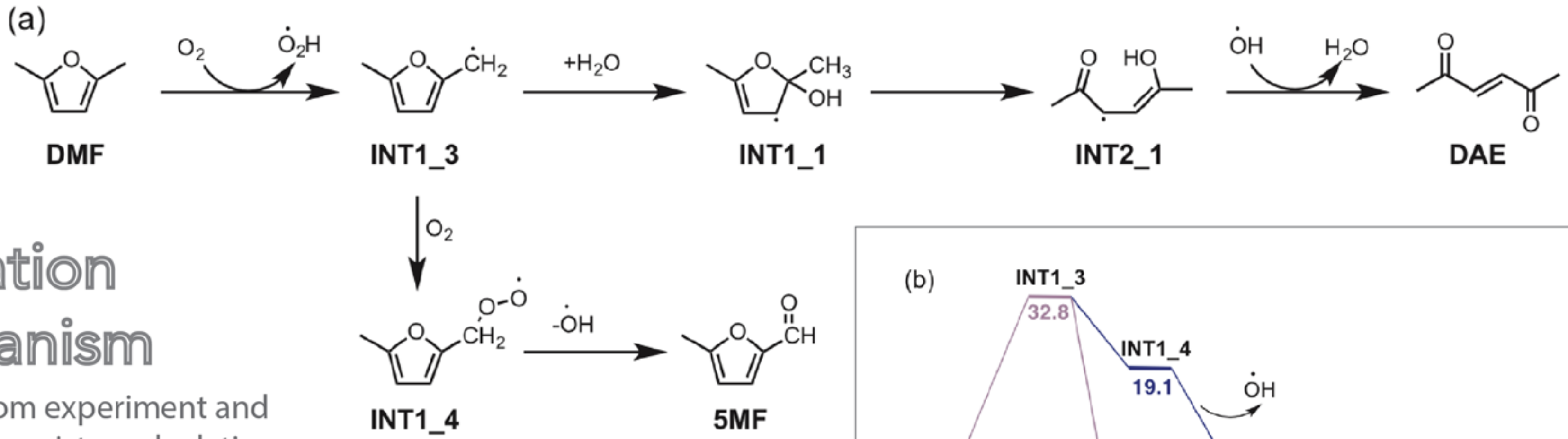
Issues

Furan blends with gasoline show poor oxidative stability, high levels of gum formation, high engine deposits, and peroxide formation

⇒ Conventional antioxidants perform poorly

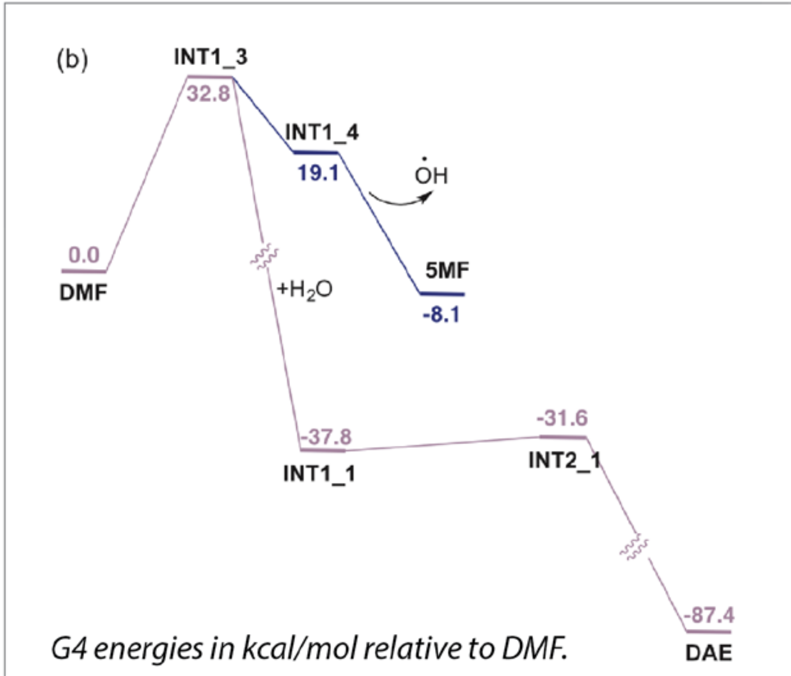


Furan Oxidation Pathways Identified



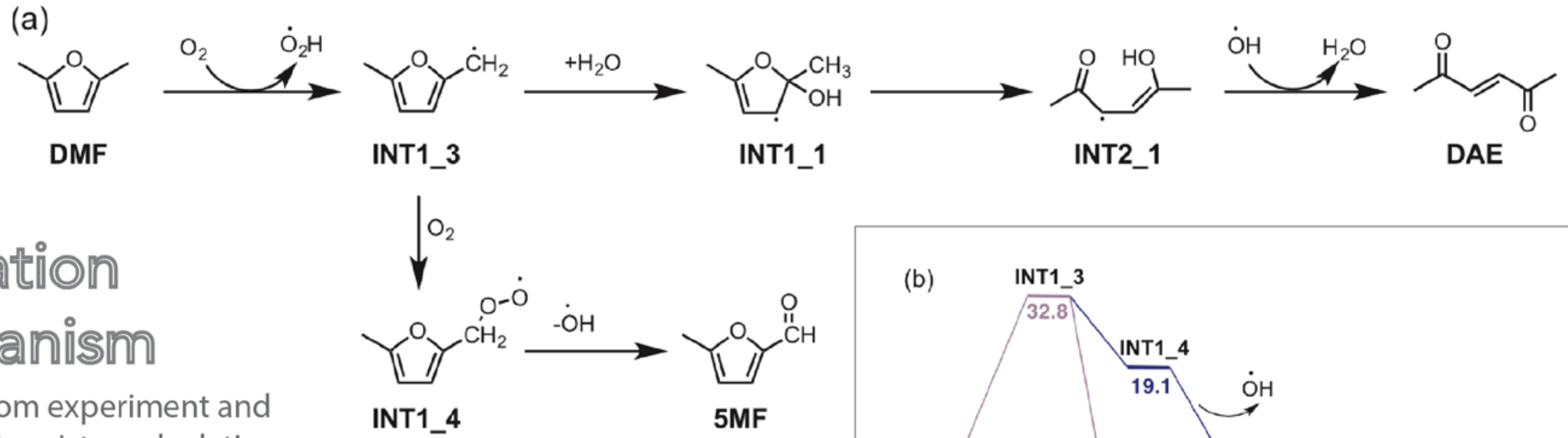
Oxidation mechanism

deduced from experiment and quantum chemistry calculations



G4 energies in kcal/mol relative to DMF.

Furan Oxidation Pathways Identified



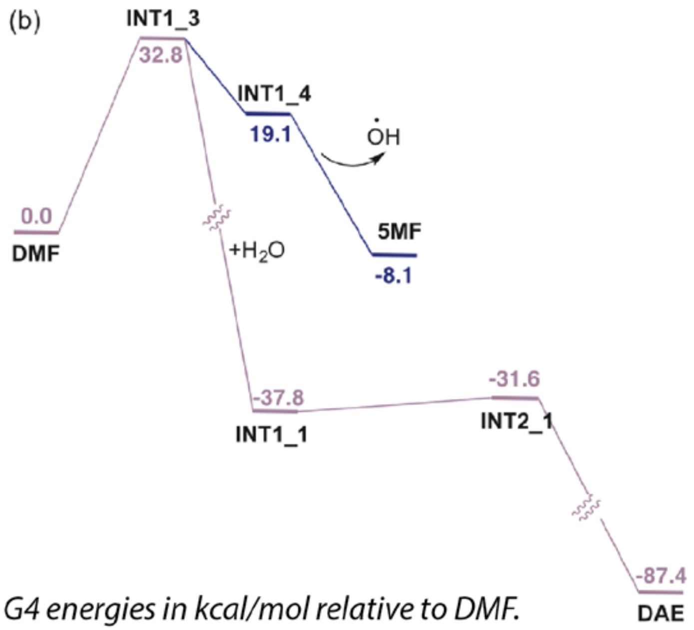
Oxidation mechanism

deduced from experiment and quantum chemistry calculations

Key insights: poor performance with standard antioxidants:

- Higher dose of furans vs "standard" gum-formers (diolefins)
- Fundamentally different oxidation chemistry - new antioxidants required to interrupt key pathways

Mechanistic understanding provides opportunity to target development of antioxidants specifically to furan reactivity



Identifying Suitable HD Diesel Bioblendstocks

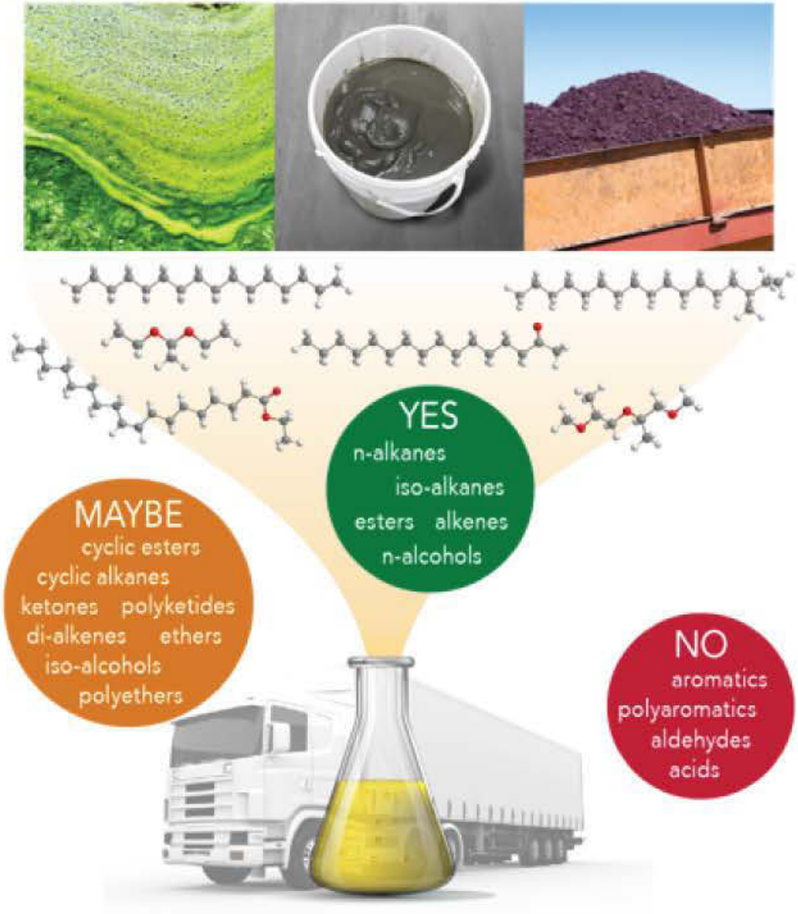
Accomplishment: Identified chemical families readily derived from biomass with properties beneficial for advanced HD diesel engines:

- Low soot formation, high CN, good cold flow properties

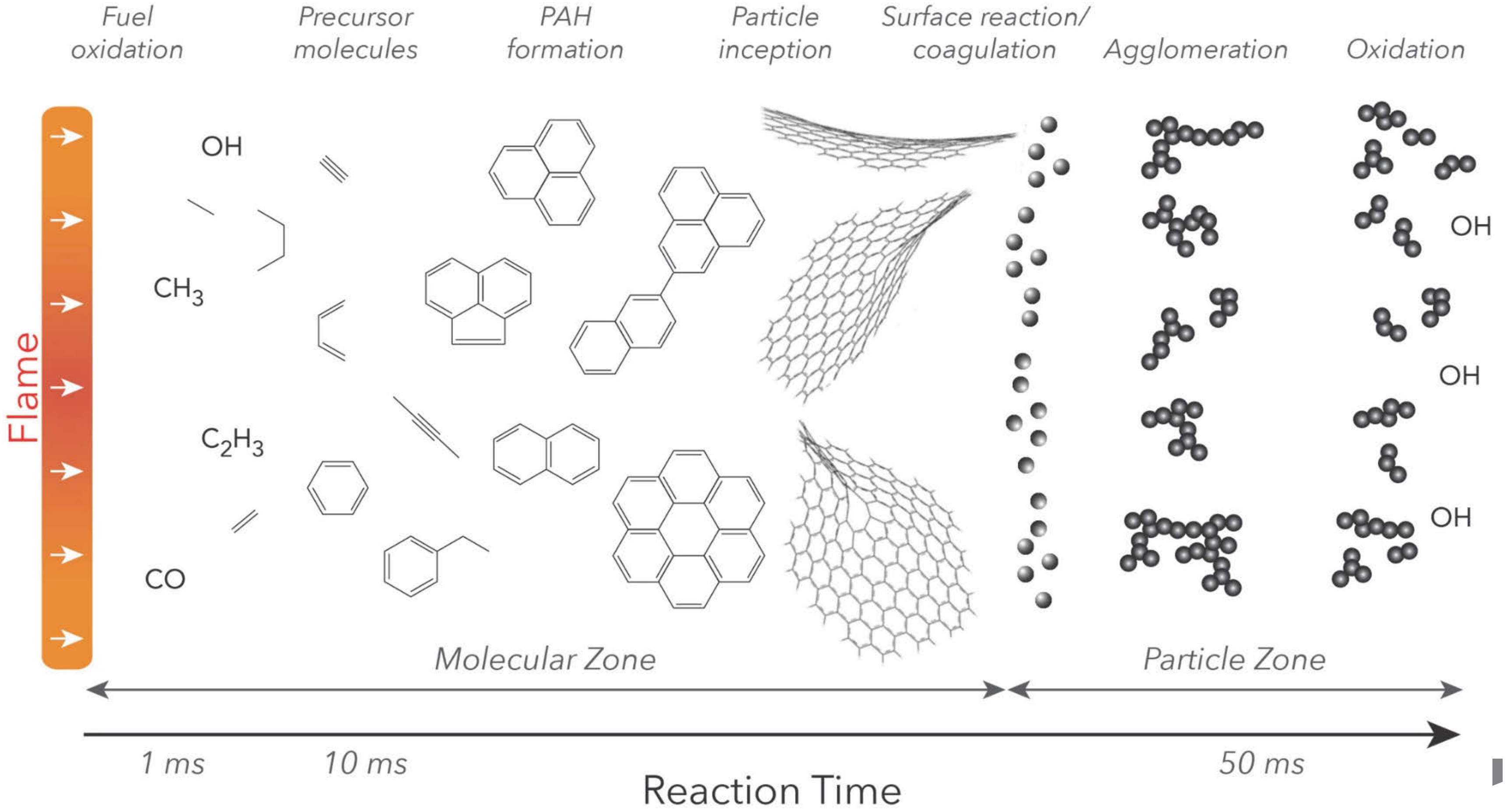
Systematic assessment identified chemical families with advantageous properties:

- Esters, alkanes, alkenes, and normal alcohols

Relevance: Results help narrow search space for high-value MCCI bioblendstocks



Predicting Soot to Guide Bioblendstock Identification



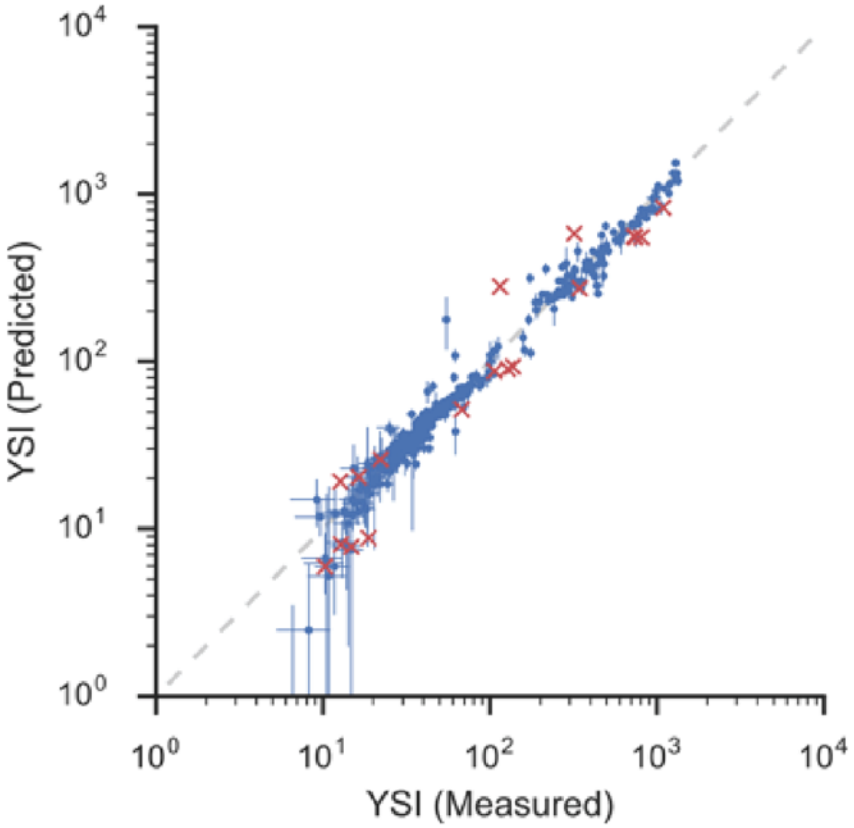
Predicting Soot to Guide Bioblendstock Identification

Predictive machine learning tool developed to rapidly estimate sooting propensity of oxygenated blendstocks

Quantitative structure–activity relationship (QSAR) model of sooting tendency based on the experimental yield sooting index (YSI)

Molecules poorly predicted by model indicate presence of complex sooting mechanisms which have been interrogated with quantum chemistry calculations

Relevance: Tool allows for rapid screening of new blendstocks on basis of sooting tendency



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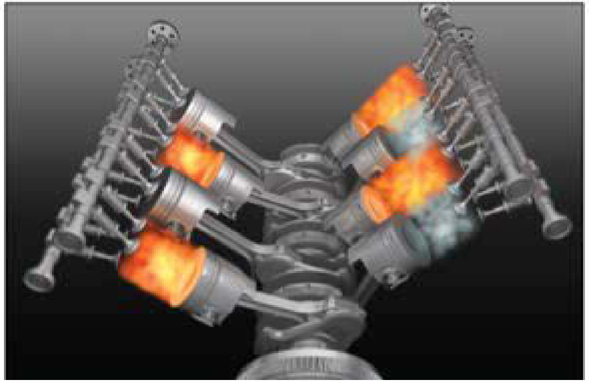

The Role of Analysis in Co-Optima

Bioblendstock Level

What are the scalability, cost, and environmental drivers?

Is a given bio-blendstock viable in the near term?

What are the key research challenges that must be overcome?

Transportation Sector Level

What will be the influence on fleet:

- Energy consumption
- Emissions – air pollutants, GHG
- Water consumption

What are potential impacts on infrastructure?

Feedstock Supply

How can companion markets build feedstock supply and what will be price impact?

Refinery Integration

What would the value proposition be to a refiner for integrating a certain bioblendstock?

Goal: Identify Key Bioblendstock Research Challenges

Technology Readiness

State of technology: Fuel production

State of technology: Vehicle use

Conversion technology readiness level

Feedstock sensitivity

Process robustness

Feedstock quality

# of viable pathways

Environmental

Carbon efficiency

Target yield

Life cycle greenhouse gas emissions

Life cycle water

Life cycle fossil energy use

Economics

Target cost

Needed cost reduction

Co-product economics

Feedstock cost

Alternative high-value use

Other Factors

Regulatory requirements

Geographic factors

Vehicle compatibility

Infrastructure compatibility

Assessed only for blendstocks produced from biomass (Technology Readiness, Environmental, Economics)

Assessed for both fossil and renewable blendstocks (Other Factors)

Summary

- Co-Optima research and analysis have identified fuel properties that enable advanced LD and HD engines
- There are a large number of blendstocks readily derived from biomass that possess beneficial properties
- Key research needs have been identified for performance, technology, economic, and environmental metrics

Thank You!